Institute for Problems in Mechanical Engineering RAS
Laboratory for "Discrete Models in Mechanics"

# Thermo-mechanical effects in perfect crystals with arbitrary multibody potential

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**Part II**: Theory. Discrete system ⟶ continuum

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# Part I Introduction

# Physical phenomenon related to thermal motion

- **thermal expansion** (*linear, nonlinear*)
- **heat conduction**
- **dissipation**
- **phase transitions** (*melting, transitions in Fe, ect.*)
- **equations of state** (*Mie-Gruneisen, etc.*)
- **wave propagation** (*elastic waves, shocks*)

# Methods for description of thermal motion

- **Phenomenological approach** (*classical thermodinamics*)

- **Statistical approaches** (*statistical physics*)

- **Molecular dynamics**

  The only method which takes thermal motion into account **explicitly**!

# Molecular dynamics

Newtonian equations of motion

$$m\ddot{\underline{r}}_i = \sum_i \underline{F}_{ij} + \underline{F}_{external}$$

$$i = 1 \ldots N$$

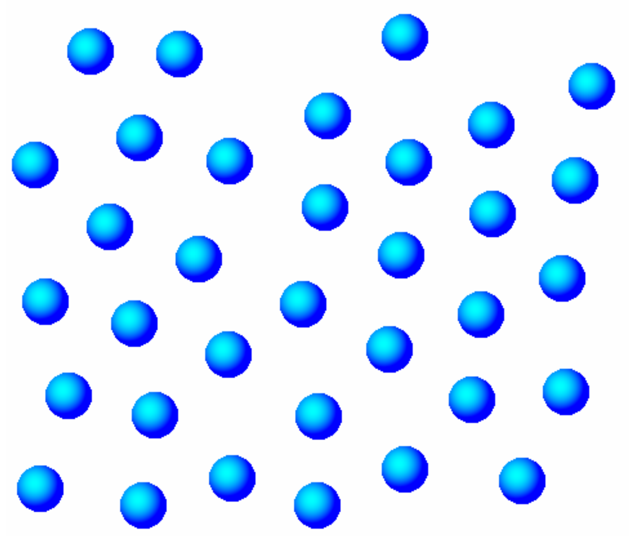
$+$

Initial conditions, constraints

numerical solution

**Results**

$$\underline{r}_i(t), \dot{\underline{r}}_i(t), \underline{F}_{ij}(t), \ldots \quad i = 1 \ldots N$$

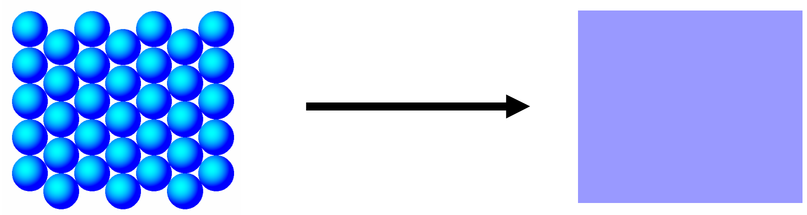


Interpretation ?

Comparison with experimental data ?

Connection with thermodynamics ?

# Part II Theory



discrete system continuum

# Different approaches

- **Smooth particle approach**

  R.J. Hardy Journal of Chemical Physics, (1982).
  J.A. Zimmerman, et. all, Modelling Simul. Mater. Sci. Eng. (2004)
  W.G. Hoover, "Smooth particle applied mechanics", World Scientific, 2006.

- **Thermo-mechanically equaivalent continuum (TMEC)**

  M. Zhou. Proc. R. Soc. A (2003)
  M. Zhou. Proc. R. Soc. A (2005).

- **Long-wave approach**

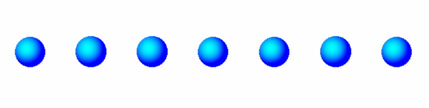
  M. Born, K. Huang, Dynamical theory of crystal lattices (1988).
  A.M. Krivtsov. "Deformation and fracture of bodies with microstructure". M., (2007).
  A.M. Krivtsov, V.A. Kuzkin. Mechanics of Solids, 2009 [paper in press]

# Hypotheses

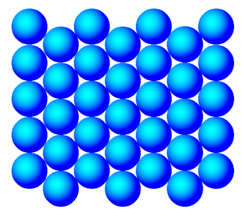
• **Structure**

Perfect crystals of simple structure are considered

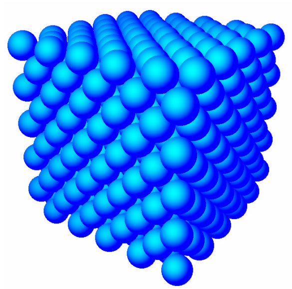
1 D



2 D



3 D



• **Discrete system** $\longrightarrow$ **Continuum**

Long wave assumption is used (Born, Huang 1988)

• **Thermal effects**

Decomposition particles' motions into continual and thermal parts is used.
The following averaging operator is applied:

$$f = \langle f \rangle + \tilde{f}, \quad \langle \tilde{f} \rangle \equiv 0$$

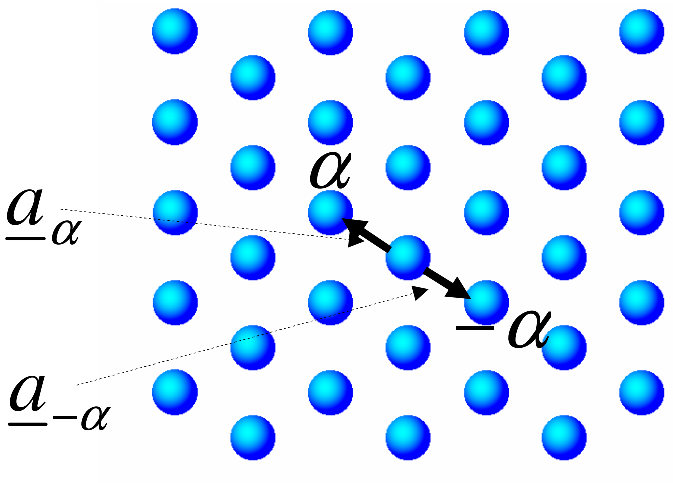
• **Interactions**

Potential energy per particle depends on all vectors connecting the given particle with its neighbors

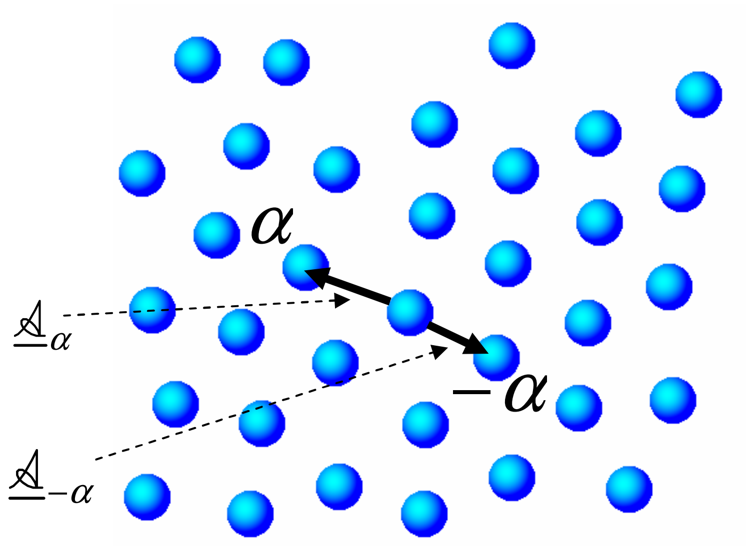
# Kinematics of discrete system and equivalent continuum

Reference configuration

$$\underline{a}_{-\alpha} = -\underline{a}_{\alpha}$$




Actual configuration




Connection with displacements of particles

$$\underline{\mathcal{A}}_\alpha = \underline{A}_\alpha + \underline{\tilde{A}}_\alpha, \quad \underline{A}_\alpha = \underline{a}_\alpha + \underline{u}_\alpha - \underline{u}, \quad \underline{\tilde{A}}_\alpha = \underline{\tilde{u}}_\alpha - \underline{\tilde{u}}$$

Connection with deformation measures

$$\underline{A}_\alpha = \underline{R}(\underline{r} + \underline{a}_\alpha) - \underline{R}(\underline{r}) \approx \underline{a}_\alpha \cdot \overset{0}{\nabla} \underline{R},$$

$$\underline{R}(\underline{r}) = \underline{r} + \underline{u}$$

Long-wave assumption

$$\boxed{A_\alpha^{\ 2} = \underline{a}_\alpha \underline{a}_\alpha \cdot\cdot \underline{\underline{G}} \qquad \underline{\underline{G}} = \overset{0}{\nabla} \underline{R} \cdot \left(\overset{0}{\nabla} \underline{R}\right)^T}$$

Cauchy-Green measure

# Interactions

Let us assume that potential energy per particle depends all vectors $\underline{a}_\alpha$

$\boxed{\Pi = \Pi\left(\left\{\underline{a}_\alpha\right\}_{\alpha\in\Lambda}\right)}$ where $\Lambda$ is a set of all particles

## Particular cases

- **Pair potentials**

$$\Pi = \frac{1}{2}\sum_\alpha \varphi(|\,a_\alpha\,|), \quad a_\alpha = |\,\underline{a}_\alpha\,|$$

- **EAM-like potential**

$\Pi = \psi\left(\sum_\alpha \rho_E(|\,a_\alpha\,|)\right)$, $\psi$ - embedding function, $\rho_E$ - electron density

- **Tersoff-like potentials** (energy depends on angles between bonds)

$$\Pi = \psi\left(\left\{\underline{a}_\alpha \cdot \underline{a}_\beta\right\}_{\alpha,\beta\in\Lambda}\right)$$

# Balance of momentum. Potential of the general type

Equation of motion of the reference particle

$$m\underline{\ddot{u}}_t = -\frac{\partial}{\partial \underline{u}_t}\left(\Pi + \sum_\alpha \Pi_\alpha\right), \qquad \Pi_\alpha = \Pi\left(\left\{\underline{\mathcal{A}}_\beta(\underline{r}+\underline{a}_\alpha)\right\}_{\beta\in\Lambda}\right)$$

Calculating the derivatives one can obtain

$$m\underline{\ddot{u}}_t = \sum_\alpha \underline{\Phi}_\alpha, \quad \underline{\Phi}_\alpha = \frac{1}{2}\left(\underline{F}_\alpha(\underline{r}) - \underline{F}_{-\alpha}(\underline{r}+\underline{a}_\alpha)\right), \quad \underline{F}_\alpha = 2\frac{\partial \Pi}{\partial \underline{\mathcal{A}}_\alpha}$$

Here $\underline{\Phi}_\alpha$ is force acting between two particles $\underline{\Phi}_{-\alpha}(\underline{r}) = -\underline{\Phi}_\alpha(\underline{r}-\underline{a}_\alpha)$

Long wave assumption $\Rightarrow$ $$m\underline{\ddot{u}} = \sum_\alpha \langle \underline{\Phi}_\alpha \rangle = \frac{1}{2}\sum_\alpha \langle \underline{F}_\alpha(\underline{r}) - \underline{F}_\alpha(\underline{r}-\underline{a}_\alpha)\rangle \approx \frac{1}{2}\sum_\alpha \left\langle \underline{a}_\alpha \cdot \overset{0}{\nabla}\, \underline{F}_\alpha \right\rangle = \overset{0}{\nabla}\cdot\left(\frac{1}{2}\sum_\alpha \underline{a}_\alpha \langle \underline{F}_\alpha \rangle\right)$$

Discrete system $$\rho_0 \underline{\ddot{u}} = \overset{0}{\nabla}\cdot\left(\frac{1}{2V_0}\sum_\alpha \underline{a}_\alpha \langle \underline{F}_\alpha \rangle\right)$$

Continuum $$\rho_0 \underline{\ddot{u}} = \overset{0}{\nabla}\cdot \underline{\underline{P}}$$

$\Rightarrow$ $$\underline{\underline{P}} = \frac{1}{2V_0}\sum_\alpha \underline{a}_\alpha \langle \underline{F}_\alpha \rangle$$ **Piola stress tensor**

Similarly in the actual configuration $$\underline{\underline{\tau}} = \frac{1}{2V}\sum_\alpha \underline{A}_\alpha \langle \underline{F}_\alpha \rangle$$ **Cauchy stress tensor**

# Comparison with known expressions for Cauchy stress tensor

- Hardy, Zimmerman $$\underline{\underline{\tau}}_{H,Z} = \frac{1}{2V}\sum_{\alpha}\left\langle \underline{A}_{\alpha}\underline{F}_{\alpha}\right\rangle - \rho\left\langle \underline{\dot{\tilde{u}}}\,\underline{\dot{\tilde{u}}}\right\rangle$$
- Zhou $$\underline{\underline{\tau}}_{Zhou} = \frac{1}{2V}\sum_{\alpha}\left\langle \underline{A}_{\alpha}\underline{F}_{\alpha}\right\rangle$$
- Krivtsov, Kuzkin $$\underline{\underline{\tau}}_{K,K} = \frac{1}{2V}\sum_{\alpha}\underline{A}_{\alpha}\left\langle \underline{F}_{\alpha}\right\rangle$$

Using equation of motion one can show that

$$\rho\left\langle \underline{\tilde{u}}\,\underline{\dot{\tilde{u}}}\right\rangle^{\cdot} - \rho\left\langle \underline{\dot{\tilde{u}}}\,\underline{\dot{\tilde{u}}}\right\rangle = \underline{\underline{\tau}}_{K,K} - \frac{1}{2V}\sum_{\alpha}\left\langle \underline{A}_{\alpha}\underline{F}_{\alpha}\right\rangle + \frac{1}{2V}\sum_{\alpha}\underline{a}_{\alpha}\cdot\overset{0}{\nabla}\left\langle \underline{\tilde{u}}_{\alpha}\underline{\tilde{F}}_{\alpha}\right\rangle$$

$$\Downarrow$$

Then in the stationary case $\boxed{\underline{\underline{\tau}}_{Krivtsov,Kuzkin} = \underline{\underline{\tau}}_{Hardy,Zimmerman}}$

# Balance of energy

Let volumetrical forces and volumetrical heat sources are absent.
The specific total energy per unit volume in the reference configuration has form

$$\rho_0 \mathcal{E} = \left\langle \frac{1}{2}\rho_0 (\underline{v} + \underline{\tilde{v}})^2 + \frac{1}{2V_0} \sum_{\alpha} \Pi\left(\{\underline{A}_\alpha\}_{\alpha\in\Lambda}\right) \right\rangle$$

Calculating the derivative with respect to time one can obtain

For discrete system $$\rho_0 \dot{\mathcal{E}} = \overset{0}{\nabla}\cdot\left(\underline{\underline{P}}\cdot\underline{v}\right) + \overset{0}{\nabla}\cdot\left(\frac{1}{2V_0}\sum_{\alpha} \underline{a}_\alpha \left\langle \underline{\tilde{F}}_\alpha \cdot \underline{\dot{\tilde{u}}}_\alpha \right\rangle\right)$$

For continuum $$\rho_0 \dot{\mathcal{E}} = \overset{0}{\nabla}\cdot\left(\underline{\underline{P}}\cdot\underline{v}\right) - \overset{0}{\nabla}\cdot\underline{h}$$

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Heat flux related
to the reference configuration

$$\underline{h} = -\frac{1}{2V_0}\sum_{\alpha} \underline{a}_\alpha \left\langle \underline{\tilde{F}}_\alpha \cdot \underline{\dot{\tilde{u}}}_\alpha \right\rangle$$

Heat flux related
to the actual configuration

$$\underline{H} = -\frac{1}{2V}\sum_{\alpha} \underline{A}_\alpha \left\langle \underline{\tilde{F}}_\alpha \cdot \underline{\dot{\tilde{u}}}_\alpha \right\rangle$$

# Constitutive relations for heat flux

Let us consider small thermal oscillations in free crystal. In this case

$$\underline{H} \approx \underline{h}, \quad \underline{A}_\alpha \approx \underline{a}_\alpha$$

Expanding heat flux with respect to $\underline{\tilde{A}}_\alpha$ one can obtain

$$\underline{H} = \nabla \cdot \left( \frac{1}{2} \sum_\alpha \underline{a}_\alpha \, {}^3\underline{\underline{C}}_\alpha \cdot\cdot \langle \underline{\tilde{u}}\underline{\tilde{u}} \rangle^{\bullet} \right) - \sum_\alpha {}^3\underline{\underline{C}}_\alpha \cdot\cdot \langle \underline{\tilde{u}}\underline{\dot{\tilde{u}}}_\alpha \rangle^S$$

Kinetic definition of the temperature $dkT = m \langle \underline{\dot{\tilde{u}}}^2 \rangle$

Expanding temperature into the same series and leaving only first order terms one obtains

$$\begin{cases} \underline{H} = \nabla \cdot \left( \frac{1}{2} \sum_\alpha \underline{a}_\alpha \, {}^3\underline{\underline{C}}_\alpha \cdot\cdot \langle \underline{\tilde{u}}\underline{\tilde{u}} \rangle^{\bullet} \right) - \sum_\alpha {}^3\underline{\underline{C}}_\alpha \cdot\cdot \langle \underline{\tilde{u}}\underline{\dot{\tilde{u}}}_\alpha \rangle^S \\ dkT = \frac{1}{2} m \underline{\underline{E}} \cdot\cdot \langle \underline{\tilde{u}}\underline{\tilde{u}} \rangle^{\bullet\bullet} + V_0 \sum_\alpha \frac{1}{a^2} \underline{a}_\alpha \cdot {}^3\underline{\underline{C}}_\alpha \cdot\cdot \langle \underline{\tilde{u}}\underline{\tilde{A}}_\alpha \rangle \end{cases}$$

**Constitutive parameters** $\langle \underline{\tilde{u}}\underline{\tilde{u}} \rangle^S, \langle \underline{\tilde{u}}\underline{\tilde{u}}_\alpha \rangle^S, \langle \underline{\tilde{u}}\underline{\dot{\tilde{u}}}_\alpha \rangle^S$

# Part II
# Applications: Equations of state. Waves propagation

## **Equations of state**. "Cold" and "thermal" components.

Let us represent $\underline{\underline{\tau}}$ and $U$ as a sum of two components

$$\rho U = \rho U_0(\overset{0}{\nabla}\underline{R}) + \rho U_T \qquad \underline{\underline{\tau}} = \underline{\underline{\tau}}_0(\overset{0}{\nabla}\underline{R}) + \underline{\underline{\tau}}_T(\overset{0}{\nabla}\underline{R}, U_T)$$

Connection with micro paramaters

$$\rho U_0 = \frac{1}{2V}\sum_\alpha \Pi(\underline{A}_a), \quad \rho U_T = \left\langle \frac{1}{2}\rho\dot{\underline{\tilde{u}}}^2 + \frac{1}{2V}\sum_\alpha \left[\Pi(\underline{A}_a + \underline{\tilde{A}}_a) - \Pi(\underline{A}_a)\right]\right\rangle$$

$$\underline{\underline{\tau}}_0 = \frac{1}{2V}\sum_\alpha \underline{A}_\alpha \underline{F}_\alpha(\underline{A}_\alpha), \quad \underline{\underline{\tau}}_T = \frac{1}{2V}\sum_\alpha \underline{A}_\alpha \left(\langle \underline{F}_\alpha\rangle - \underline{F}_\alpha(\underline{A}_\alpha)\right)$$

Equation of state for cold components was derived in the book
A.M. Krivtsov "Deformation and fracture of bodies with microstructure"

$$\rho U_0 = \frac{1}{2V}\sum_\alpha \Pi(|\underline{a}_\alpha \cdot \overset{0}{\nabla}\underline{R}|),$$

$$\underline{\underline{\tau}}_0 = \frac{1}{2V}\left(\underline{R}\overset{0}{\nabla}\right) \cdot \sum_\alpha \underline{a}_\alpha \underline{F}_\alpha(\underline{a}_\alpha \cdot \overset{0}{\nabla}\underline{R})$$

# Equation of state for *thermal* components

Let us expand the following expressions into series with respect to $\underline{\tilde{A}}_a$

$$\underline{\underline{\tau}}_T = \frac{1}{2V}\sum_\alpha \underline{A}_\alpha \left(\left\langle \underline{F}_\alpha \right\rangle - \underline{F}_\alpha(\underline{A}_\alpha)\right)$$

$$\rho U_T = \left\langle \frac{1}{2}\rho \dot{\underline{\tilde{u}}}^2 + \frac{1}{2V}\sum_\alpha \left[\Pi(\underline{A}_a + \underline{\tilde{A}}_a) - \Pi(\underline{A}_a)\right]\right\rangle$$

Thereto let us use the expression

$$\underline{F}_\alpha(\underline{A}_\alpha + \underline{\tilde{A}}_\alpha) = \underline{F}_\alpha(\underline{A}_\alpha) + \sum_{n=1}^{\infty} {}^{n+1}\underline{\underline{F}}_\alpha \odot {}^{n}\underline{\underline{\tilde{A}}}_\alpha, \quad {}^{n+1}\underline{\underline{F}}_\alpha = \frac{1}{n!}\frac{d^n \underline{F}_\alpha}{d\underline{A}_\alpha^n}, \quad {}^{n}\underline{\underline{\tilde{A}}}_\alpha = \overset{n}{\otimes}\underline{\tilde{A}}_\alpha$$

As a result assuming that $\left\langle {}^{2n+1}\underline{\underline{\tilde{A}}}_\alpha \right\rangle = 0$ one obtains

$$\underline{\underline{\tau}}_T = \frac{1}{2V}\sum_\alpha \sum_{n=1}^{\infty} \underline{A}_\alpha \, {}^{2n}\underline{\underline{F}}_\alpha \odot \left\langle {}^{2n}\underline{\underline{\tilde{A}}}_\alpha \right\rangle$$

$$\rho U_T = \frac{1}{4V}\sum_\alpha \sum_{n=1}^{\infty} \frac{n+1}{n} \, {}^{2n}\underline{\underline{F}}_\alpha \odot \left\langle {}^{2n}\underline{\underline{\tilde{A}}}_\alpha \right\rangle$$

**Constitutive parameters**

$$\left\langle {}^{2n}\underline{\underline{\tilde{A}}}_\alpha \right\rangle, \quad n = 1..\infty$$

# Mie–Gruneisen equation of state

$$p_T = \frac{\Gamma(V)}{V} U_T$$

- $p_T$ – thermal pressure

$p_T = -\frac{1}{d}\mathrm{tr}(\underline{\underline{\tau}}) - p_0$, where $d$ - dimension (1,2 or 3)

$p_0 = -\frac{1}{d}\mathrm{tr}(\underline{\underline{\tau}})\,|_{\tilde{A}_\alpha = 0}$ - ‘cold’ pressure

- $U_T$ – thermal energy
- $V$ – specific volume
- $\Gamma(V)$ – Gruneisen’s coefficient

# First approximation. Generalized Mie-Gruneisen EOS

Let us leave only first nontrivial terms in the expansions, then

$$\underline{\underline{\tau}} = -\frac{1}{2V}\sum_{\alpha}\left[\Phi' \underline{A}_{\alpha}\underline{A}_{\alpha}\underline{\underline{E}} + 2\Phi' \underline{A}_{\alpha}\underline{\underline{E}}\underline{A}_{\alpha} + 2\Phi'' \underline{A}_{\alpha}\underline{A}_{\alpha}\underline{A}_{\alpha}\underline{A}_{\alpha}\right]\cdot\cdot\left\langle \underline{\tilde{A}}_{\alpha}\underline{\tilde{A}}_{\alpha}\right\rangle$$

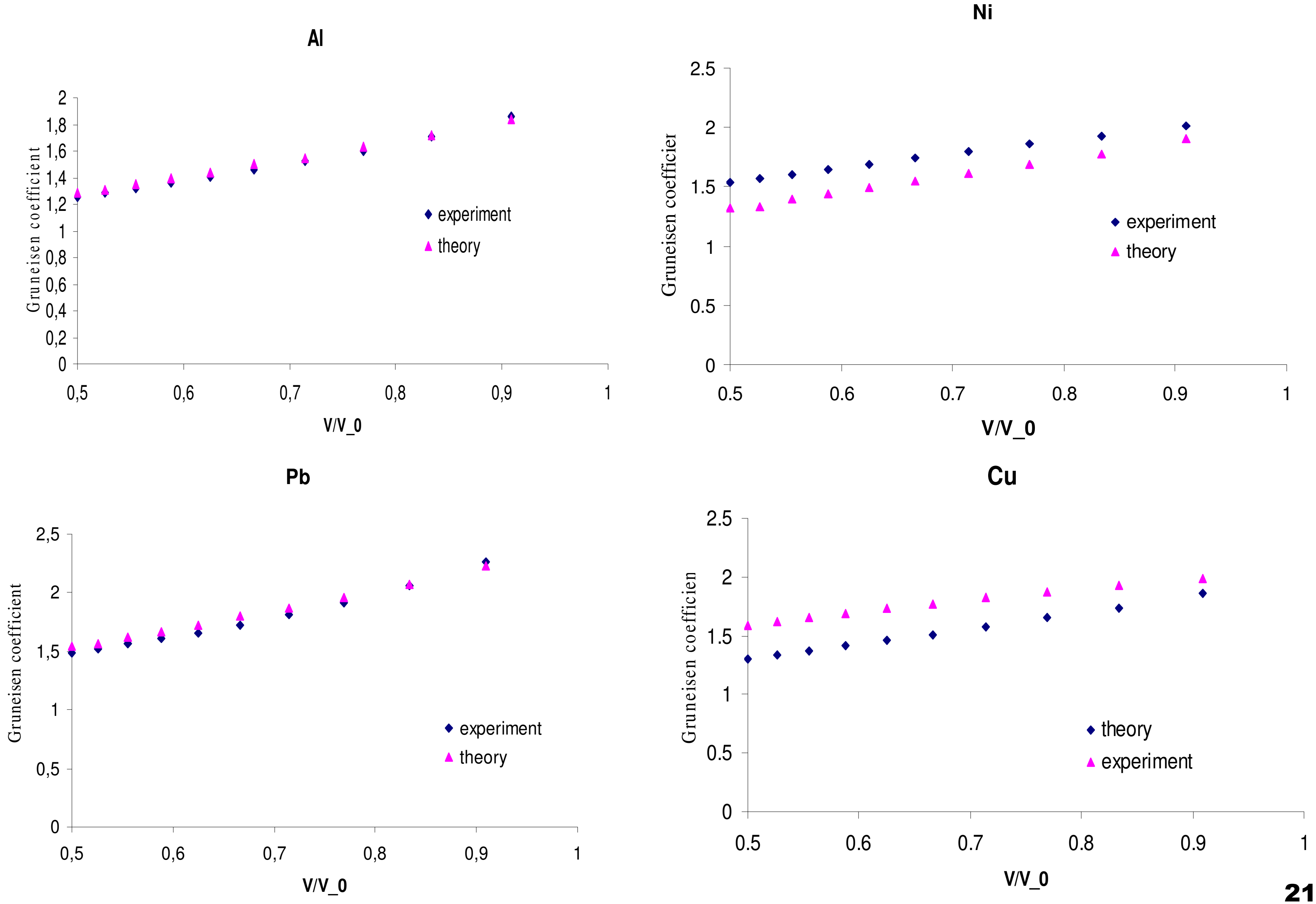
$$\rho U_T = -\frac{1}{2V}\sum_{\alpha}\left(\Phi \underline{\underline{E}} + 2\Phi' \underline{A}_{\alpha}\underline{A}_{\alpha}\right)\cdot\cdot\left\langle \underline{\tilde{A}}_{\alpha}\underline{\tilde{A}}_{\alpha}\right\rangle,$$

Assume that $\left\langle \underline{\tilde{A}}_{\alpha}\underline{\tilde{A}}_{\alpha}\right\rangle = \eta \underline{\underline{E}}$

Then the generalized Mie-Gruneisen EOS has the following form

$$\underline{\underline{\tau}}_T = \underline{\underline{\Gamma}}\rho U_T, \qquad \underline{\underline{\Gamma}} = \frac{\sum_{\alpha}\left((d+2)\Phi' A_{\alpha} + 2\Phi'' A_{\alpha}^2\right)\underline{A}_{\alpha}\underline{A}_{\alpha}}{\sum_{\alpha}\left(d\Phi + 2\Phi' A_{\alpha}^2\right)}$$

# Gruneisen function: comparison with the experimental data



# Second approximation. Nonlinear EOS

Expanding $p_T, U_T$ into series, leaving only terms of order of $\left\langle \underline{\tilde{A}_\alpha} \underline{\tilde{A}_\alpha} \underline{\tilde{A}_\alpha} \underline{\tilde{A}_\alpha} \right\rangle$

and assuming that $\left\langle \underline{\tilde{A}_\alpha} \underline{\tilde{A}_\alpha} \underline{\tilde{A}_\alpha} \underline{\tilde{A}_\alpha} \right\rangle = \dfrac{\lambda \eta^2}{d(d+2)} \left( \underline{\underline{E}}\,\underline{\underline{E}} + \underline{e}_n \underline{\underline{E}}\,\underline{e}_n + \underline{e}_n \underline{e}_k \underline{e}_n \underline{e}_k \right)$

One can obtain the following system connecting pressure and thermal energy

$$\begin{cases} p_T = f_1 \eta + f_2 \lambda \eta^2 \\ U_T = f_3 \eta + f_4 \lambda \eta^2 \end{cases} \qquad \lambda = \frac{\left\langle \underline{\tilde{A}_\alpha}^4 \right\rangle}{\left\langle \underline{\tilde{A}_\alpha}^2 \right\rangle^2}$$

## Nonlinear EOS

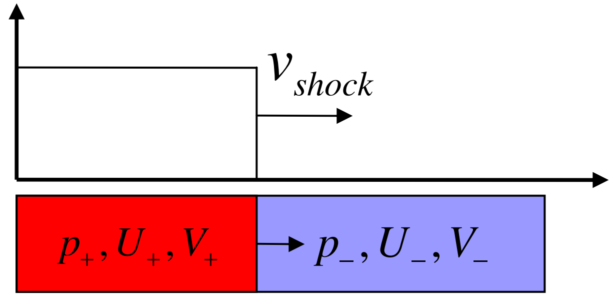
$$p_T = \frac{(f_2 f_3 - f_1 f_4)(f_3 - \sqrt{f_3^{\,2} + 4\lambda f_4 U_T})}{2\lambda f_4^{\,2}} + \frac{f_2}{f_4} U_T$$

# Hugoniot

Conservational laws

$$U_+ - U_- = \frac{1}{2}\left(p_+ + p_-\right)\left(V_- - V_+\right)$$

- Hugoniot in hydrodynamic approximation




Let $U_- = U_0(V_0), V_- = V_0,\ p_- = 0,\ p_+ = p_H, U_+ = U.$

- Hugoniot for Mie Gruneisen EOS (Glushak, Kuropatenko, 1992)

$$p_H = \frac{2p_0(V)V - 2\Gamma(V)(U_0(V) - U_0(V_0))}{2V + \Gamma(V)\,(V - V_0)}.$$

$$\exists V_* : \quad 2V_* + \Gamma(V_*)\left(V_* - V_0\right) = 0!!!$$

- Hugoniot for nonlinear EOS

$$A^2 p_H^2 + (2AB - C)p_H + B^2 + Cp_0 - f_1^2 = 0,$$

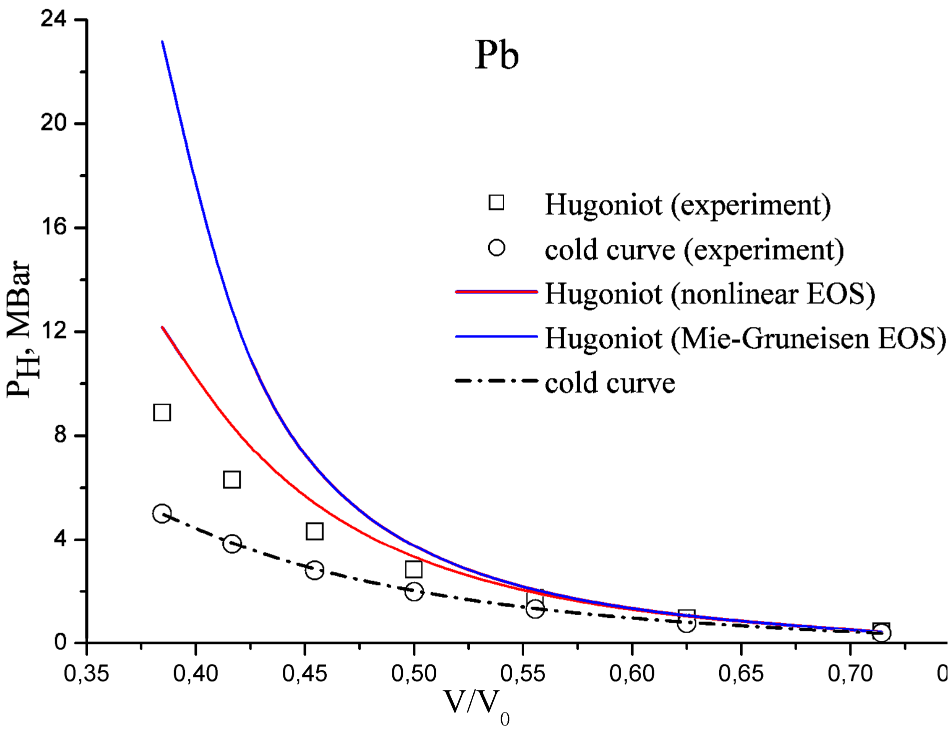
$$A = \lambda_2 f_2 \frac{f_2(V_0 - V) - 2f_4}{f_1 f_4 - f_2 f_3}, \quad B = 2\lambda_2 f_2 \frac{f_4 p_0 - f_2 U_0}{f_1 f_4 - f_2 f_3} - f_1, \quad C = 4\lambda_2 f_2.$$

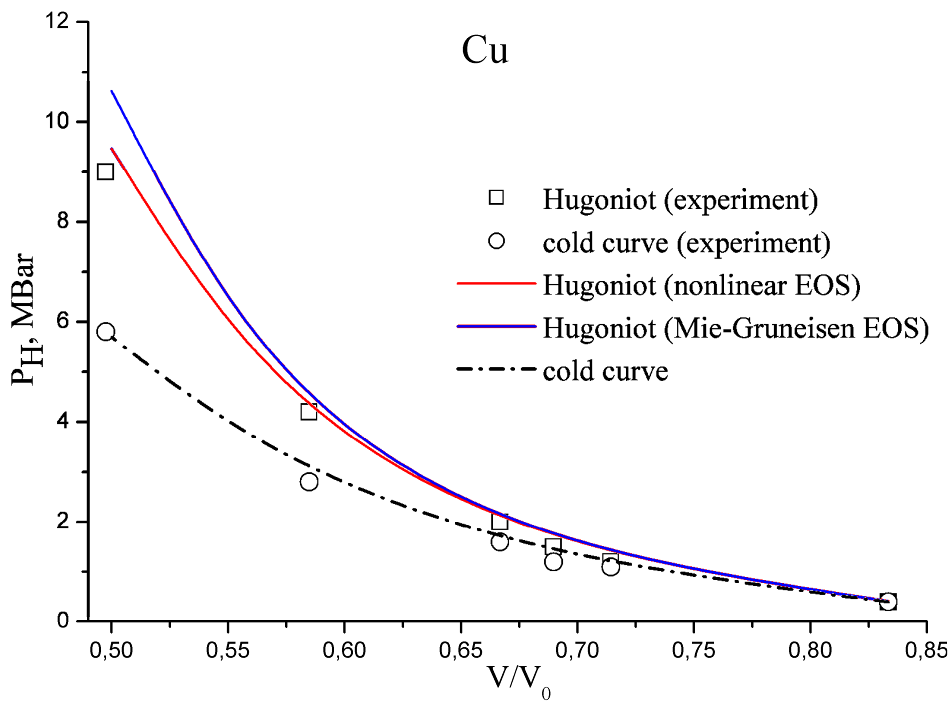
# Comparison with experimental data (Altshuller, 1965)

**Parameters of the model:**

- Morse potential (copper $\alpha a = 4.65, \frac{D}{a^3} = 0.031\,\mathrm{MBar}$, lead $\alpha a = 4.47, \frac{D}{a^3} = 0.013\,MBar$)
- Two coordination spheres

## Hugoniots and cold curves for Cu and Pb



# Nonlinear wave equation in adiabatic approximation

Let us assume that heat flux is equal to zero or constant over space

$$\rho_0 \dot{U} = \underline{\underline{P}} \cdot\cdot \left( \underline{R}\,\overset{0}{\nabla} \right)^{\bullet} \rightarrow \rho_0 (U_0 + U_T)^{\bullet} = (\underline{\underline{P}}_0 + \underline{\underline{P}}_T)\cdot\cdot\left(\underline{R}\,\overset{0}{\nabla}\right)^{\bullet}$$

$$\underline{\underline{P}}_0 = \rho_0 U_0^{\;*}$$

$$\underline{\underline{P}}_T(\overset{0}{\nabla}\underline{R}, U_T) = \rho_0 U_T^{\;*}$$

Differential equation with respect to $U_T(\overset{0}{\nabla}\underline{R})$

Hereinafter $\psi^{*} \overset{def}{=} \dfrac{d\psi}{d\,\overset{0}{\nabla}\underline{R}}$

Substituting the last expressions into equation of motion one obtains

$$\ddot{\underline{u}} = \overset{0}{\nabla}\cdot\left(U_0^{\;*} + U_T^{\;*}\right) \rightarrow \boxed{\ddot{\underline{u}} = \left(U_0^{\;*T} + U_T^{\;*T}\right)^{*} \cdot\cdot\cdot\, \underline{u}\,\overset{0}{\nabla}\,\overset{0}{\nabla}}$$

If equation of state is given in the form $\underline{\underline{P}}_T = \underline{\underline{P}}_T(\overset{0}{\nabla}\underline{R}, U_T)$ then

$$\boxed{\rho_0\,\ddot{\underline{u}} = \underline{\underline{P}}_0^{\;T*}\cdot\cdot\cdot\,\underline{u}\,\overset{0}{\nabla}\,\overset{0}{\nabla} + \left(\frac{\partial \underline{\underline{P}}_T^{\;T}}{\partial\overset{0}{\nabla}\underline{R}} + \frac{1}{\rho_0}\frac{\partial\underline{\underline{P}}_T^{\;T}}{\partial U_T}\underline{\underline{P}}_T\right)\cdot\cdot\cdot\,\underline{u}\,\overset{0}{\nabla}\,\overset{0}{\nabla}}$$

# First approximation. Uniaxial deformation

Let us consider uniaxial deformation of the medium in direction $\underline{e}$

$$\underline{R} = \underline{r} + u(\underline{r}\cdot\underline{e}, t)\underline{e} \quad \Rightarrow \quad \overset{\circ}{\nabla}\underline{R} = \underline{\underline{E}} + u'\underline{e}\underline{e}, \quad u' \overset{\text{def}}{=} \frac{\partial u(\underline{r}\cdot\underline{e}, t)}{\partial(\underline{r}\cdot\underline{e})}.$$

Then equation of balance of energy takes form

$$\frac{d\mathcal{U}_T}{du'}\underline{e}\underline{e} = \underline{\underline{\Gamma}}_0\mathcal{U}_T. \Rightarrow \quad \mathcal{U}_T = \mathcal{U}_T^0 \exp\left(\underline{e}\underline{e}\cdot\cdot\int_{u'_0}^{u'}\underline{\underline{\Gamma}}_0(u')du'\right)$$

As a result one can obtain closed wave equation

$$\boxed{\rho\ddot{u} = \frac{V_0}{V}\left[\frac{d\underline{\underline{\tau}}_0}{du'}\cdot\cdot\underline{e}\underline{e} + \rho\frac{V_0}{V}\mathcal{U}_T^0 \exp\left(-\int_{u'_0}^{u'}\frac{\Gamma}{1+u'}du'\right)\left(\Gamma^2 + \Gamma - \frac{V}{V_0}\Gamma'\right)\right]u'', \quad \frac{V}{V_0} = 1+u'.}$$

In the case $|u'| \ll 1$ one obtains linear wave equation

$$\boxed{\ddot{u} = v_l^2 u'', \qquad v_l^2 \overset{\text{def}}{=} \frac{1}{\rho_0}\left[\frac{d\underline{\underline{\tau}}_0}{du'}\cdot\cdot\underline{e}\underline{e} + \underline{\rho_0\mathcal{U}_T^0\left(\Gamma^2 + \Gamma - \Gamma'\right)}\right]}$$

the influence of thermal motion

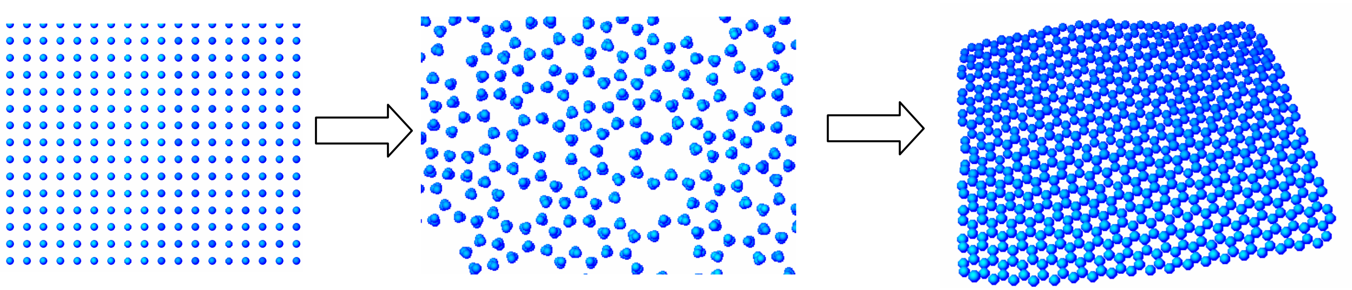
# Results

- ✓ The generalization of approach for transition from discrete system to equivalent continuum in the case of potential of he general type is conducted
- ✓ Expressions connecting stress tensors with parameters of microstructure are obtained
- ✓ Comparison with known expressions for Cauchy stress tensor is conducted
- ✓ Approach for equations of state obtaining is generalized for 3D case
- ✓ Equations of state in Mie-Gruneisen form and more general nonlinear form are obtained
- ✓ Comparison with experimental data is presented

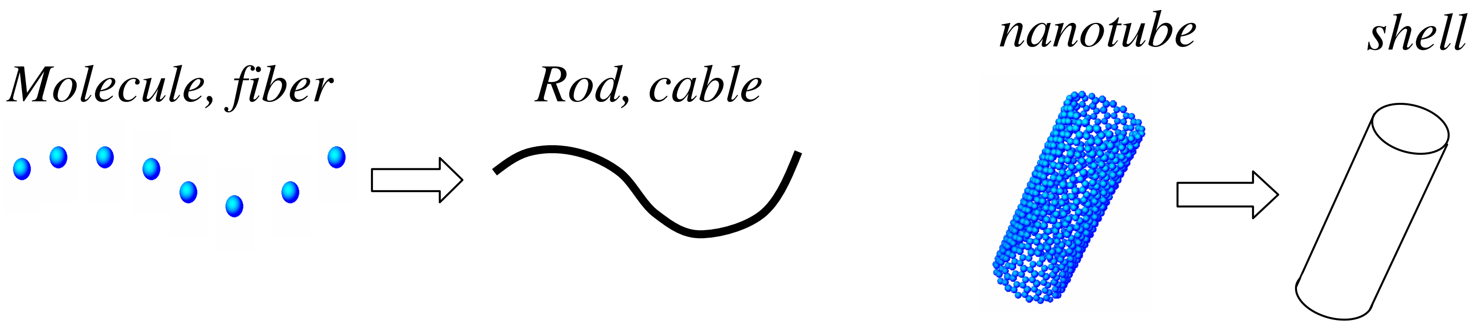
# Future work

1) Macroscopic dissipation ⟺ thermal motion

2) Modeling of creation of carbonic materials



3) Continualization of rod-like and shell-like nano structures




4) Identification of residual stresses using TSA technique

Thank you for your attention !